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PROBLEM-SOLVING PROCESSES USED BY GRADUATE STUDENTS WHILE SOLVING TASKS IN ORGANIC SYNTHESIS

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Problem solving is a complex set of behaviors that has been described by information-processing models such as the one proposed by Bourne, Dominowski and Loftus (1979). They view problem solving as a non-linear, three-stage process.

Preparation is the first stage. During this stage the problem solver interprets the problem and begins to construct a representation of it. They concluded:

> The outcome of preparation is an interpretation of the problem, a representation of the problem as seen by the person who must try to solve it. The nature of a person's interpretation is an important determinant of how readily the problem will be solved.... In addition, individuals differ in the kinds of representations they construct, with definite effects on their chances of success. (p. 239)

The representation that is constructed during the preparation phase is used in the production stage.

Production is the second stage. The problem solver begins constructing a solution based on the representation constructed in the first stage and the knowledge he or she brings to the problem.

Evaluation is the third stage of the model. During this stage the solution is evaluated for its completeness and correctness. Bourne et al. conclude the following about the importance of the evaluation stage:

> It should be clear that, for many problems, a person may fail to solve a problem, take a long time in doing so, or even arrive at a poor quality solution not because of inadequate production of ideas but because of inadequate evaluation of those ideas. (p. 243)

These stages of problem solving — preparation, production, and evaluation — have been presented as a linear sequence of events. Bourne et al. contend that for complex problems the process is not linear. Problem solvers might switch back and forth between all of these stages as their needs change.

> Logically, it would seem that preparation is the first step, production the second, and judgment the third. However, complex problem solving generally involves considerable recycling through these stages. For example, a person

> trying out one idea after another is cycling repeatedly through production and judgment. When evaluation leads to the decision that production is proving fruitless, a person might well reenter the preparation stage to try developing a different interpretation of the problem. Also, if there is a great amount of problem information to be assimilated, a person might forget some of it and return for this reason to the preparation stage. (p. 239)

Related Research

Most research that has been done on problem solving in science can be related to the first two stages of the model described above. Unfortunately not much research has been done examining how problem solvers evaluate their solution (unless the evaluation is considered a subset of the production stage). The purpose of this section is to describe some of the research relevant to this model and the purpose of this study.

In preparing to solve a problem a person constructs a representation of the problem to be solved. A representation is a dynamic structure reflecting the problem solver's understanding of the problem and the knowledge he or she brings to the problem. As the person solves the problem their understanding of the problem and the knowledge might change as they learn by solving the problem. Numerous studies have been done to examine the role of representations in problem solving while other work has examined the production of solutions.

Larkin and Reif (1979) studied representations subjects used and what subjects did while generating solutions to physics problems. They found that the expert and novice began solving the problem by constructing an external representation of the physical situation described in the problem. The novice then constructed a mathematical representation by combining equations and eliminating unknowns until the problem was solved. The expert decided what physics principles were relevant to the situation and began to construct a mathematical representation of the situation. However, instead of combining equations to eliminate unknowns, he used subsidiary principles to reduce the number of unknowns.

In the same study Larkin and Reif also designed instruction in problem solving based on their understanding of the processes their subjects displayed. They found that the expert problem solver displayed two behaviors that novices did not: 1) The expert used methods based on underlying principles, and 2) A low-detail qualitative representation was constructed to explore potential difficulties with the solution. In the second part of the study they conducted an experiment designed to investigate the effect explicit teaching of these two behaviors has on problem-solving performance. The group that was taught to use methods based on underlying principles and qualitative representations to explore difficulties performed better than the control group when asked to solve three physics problem.

Greenbowe (1984) investigated numerous variables related to successful problem solving of stoichiometry problems in general chemistry. One of the variables he examined was evaluation behaviors such as checking arithmetic or determining the reasonableness of an answer. Subjects were given one of three possible scores. Subjects that were successful solving the tasks had significantly higher evaluation scores than the unsuccessful problem solvers.

Frank (1986) commented on some of the evaluation behaviors that subjects showed when they were involved in a problem-solving instruction experiment in a general chemistry class. Experimental sections of students were taught within their recitation section to use heuristics while solving problems. Those students in the control sections were taught recitation in the traditional manner. Frank made the following comments about the evaluation behaviors the subjects displayed: "The experimental students evaluated their work during solutions more often, they evaluated their answers more often, they were more persistent, and they made fewer uncorrected math errors. (p. ?)" Although they seem to be useful qualities for problem solving, he points out "although the experimental students evaluated their work more often than the control students, they didn't do it very often. (p. ?)"

Although work has been done looking at how people construct representations, and generate and evaluate solutions for problems in physics and general chemistry, this type of work has not been examined in a non-mathematical area such as organic synthesis. Using the model of problem solving described earlier, the purpose of this paper is to describe the problem solving processes graduate students utilize while solving tasks related to organic synthesis.

Method

This section provides a description of the subjects, instruments, procedures, and methods of data collection and analysis used in this study.

Subjects, Instructor, and the Classroom

A sample was obtained by soliciting volunteers from a graduate-level synthesis course at a large university during the spring of 1987. Of the 35 students in the course about half volunteered to serve as subjects. Of these, ten were actually interviewed. Most of the subjects were graduate students pursuing the PhD in organic chemistry, although three of the subjects were from other departments. A description of the instructor's goals, classroom environment, and student evaluation procedures can be found elsewhere (Bowen, in press).

Instruments

Three instruments were developed by the researcher and piloted before the study was begun. They were designed to focus on the three stages of problem solving cited above. During the period data were being collected additional instruments were developed to investigate working hypotheses constructed from analysis of earlier protocols. Below are brief descriptions of the tasks discussed in this paper. Copies of these tasks can be found in the appendix.

Task 1: Synthesis Without Starting Material.

Task 1 was designed to provide information about subjects' strategies for the production stage of problem solving. Subjects were expected to show behaviors relevant to generating a solution. For the most part this was what occurred throughout the first few interviews. However, by asking other questions such as "Why are you choosing that target?", it became possible to also examine the preparation phase of problem solving.

Task 2: Synthesis With Starting Material.

This task was also designed to provide information about strategies subjects use for the production stage of problem solving. This task also provided a look at the preparation stage, but one that differed from task 1. This problem is a more well-defined task because the initial state is defined (i.e., the starting material is indicated).

Task 3: Structure Analysis.

This task was designed to focus on the preparation phase of problem solving. It was expected that subjects would display behaviors related to preparing to solve a synthesis problem. Subjects were expected to analyze compounds for potential difficulties, but not actually produce a synthetic pathway.

Task 4: Evaluating Syntheses.

Task 4 was developed to examine the evaluation processes subjects use while problem solving. By having subjects determine which of two syntheses is best and explain why, it was hoped that they would concentrate on the evaluation stage. A task was desired in which the chemistry was fairly straightforward, and both syntheses short. The first of these pathways is by Mori & Senda (1985), while the second pathway is found in Pirkle & Adams (1979).

Task 5: Selecting Target Structures.

This task was developed after the first three subjects had been interviewed. The following question came up after these interviews: "Why do subjects choose certain target molecules?" This task was designed to look at the preparation stage of problem solving. By asking subjects to examine potential target molecules, they might concentrate on certain aspects of the structure on which their decision was based. It became apparent after using this task, that equally useful information could be obtained from tasks 1 and 2 if subjects were asked why they picked a particular target.

Procedure

Subjects were individually interviewed by the researcher using the think aloud method. With this method subjects are given tasks and asked to describe how they are solving the task. The data consist of a transcript of each interview and written work the subject produced. For a discussion of the method and some of its pitfalls see Schoenfeld (1985).

All interviews were tape recorded for later transcription and analysis. The length of the interviews ranged from 45 to 90 minutes, with the average being about 65 minutes. The researcher attempted to make the subjects feel as comfortable as possible by providing several common organic textbooks and reference books, and a model kit. Each subject was first asked to solve a warm-up task so the researcher could provide feedback about how well he or she was "thinking aloud". Following the warm-up task, the subject was given from two to five additional tasks to solve. Each task was answered by at least four subjects and all subjects were asked to solve either task 1 or 2. The researcher stressed to the subject that he was primarily interested in *how the solution was arrived at.*

Data Analysis

Data were analyzed in three phases. First, following each interview preliminary analyses were performed to catalog behaviors the subject showed while solving the tasks. These listings provided working hypotheses about behaviors subjects might show while solving synthesis tasks that could be examined in later interviews. In the second stage of analysis trends in the behaviors a subject exhibited were used to infer processes the subject might utilize while problem solving in synthesis. An approach to problem solving for each subject was constructed through the use of these inferences. These approaches were used in the final phase of data analysis to infer general problem-solving processes that graduate students utilize while solving tasks in organic synthesis. (All excerpts are taken from Bowen, 1987 and reference the subject number and pages from the transcripts.)

Results

The purpose of this section is to provide examples of the types of behaviors subjects displayed while problem solving. Samples of preparation, production and evaluation behaviors related to synthesis are reported according to the tasks described earlier. In the final section a summary is given describing how graduate students solve problems in organic synthesis.

Preparation — Tasks 3 and 5

Subjects showed similar preparation tactics while working on these two tasks. Examination of the functional groups that were present (or lack of functionality) was usually the first step. The subjects correlated the functional groups to the target through a retroanalysis and suggested reactions that could be used to form the molecule. In addition, they decided how difficult it would be to carry out the reaction to decide what is difficult to synthesize in the target molecule. Some of the subjects evaluated the difficulty of forming a target molecule based on interactions between various functional groups in the molecule or the presence of stereochemistry.

Below are several excerpts from the transcripts that are illustrative of the processes described above.

D Well I would probably say the very bottom one [is the one to synthesize]. For one thing it's a lot simpler in that you don't have to worry about the stereochemistry. So your reactions wouldn't have to be quite so selective.

R Uh huh.

D Also a. Let's see. Why else? The the top one just doesn't have much functionality accept for the carboxylic acid.... But a the bottom one just looks -- I don't know. There there are a lot of cyclization methods for five membered rings. (s4, p. 9).

Stereochemistry was one of the first problems Dan identified with task 5. Functionality was another criterion he used to discount one of the other structures. Dan also suggested that there are several ways he might actually make the five-membered ring in the target.

A Well I have -- first looking at this one I have I'm seeing two functional groups. A the alcohol on the upper part of the molecule, and the lactone on the second part.... Well, I know as my future project include I know that lactone are quite difficult to obtain when you you want to to do them. And they are very bad yield... Uh so to figure out what the what the most difficult part of the molecule is I have to to break it down.

R Uh huh.

A Well the first part I see I have an alcohol here. And I'm breaking down the ester I have. To end up with my my acid and alcohol before esterification. So um well maybe that's the answer. This is going to be -- if I -- if this is my previous molecule, uh I mean, this molecule was made from this one, the step coming from this one to this one is going to be very difficult. Because I have two alcohols.

R Uh huh.

A And uh when I going to to try and make the lactone, even if one of these is going to make a one, two, three, four, five membered ring, and another one a six membered ring, I'm going to have both of them. And this is going to lower my yield. And it doesn't need this already. (s1, p. 11-12).

Functional groups that were present and the rated difficulty of forming them was a method Andrew used to solve task 3. He broke the molecule down to determine how the lactone might be formed in the forward direction. By breaking down the molecule Andrew saw a difficulty with two competing reactions that could occur — formation of both five and six-membered lactones from the corresponding diol.

H Definitely I won't pick the second of them. Because steric it's uh have to consider stereo

R Stereochemistry?

H Yea. Stereochemistry.

R Uh huh.

H That's much more difficult.... And uh this one -- yea this one also look quite. I cannot see through very quickly. Maybe I'll choose this one.

R Bottom one. How come?

H Because this one also.

R The stereochemistry?

H Yea. I'm scared of stereochemistry. (s8, p. 3).

Stereochemistry that was present caused Helen to reject two of the target compounds in task 5. She did not feel comfortable with stereochemistry so she avoided it.

Production — Tasks 1 and 2.

While in the production phase of problem solving the subjects used numerous tactics. Behaviors included such approaches as correlating functional groups in a target molecule with those in the starting material, using a text to locate a particular family of reactions, abandoning a solution when it appeared useless, and simplifying the task at hand.

Below are excerpts from the protocols that are illustrative of the behaviors subjects displayed while in the production phase.

A ... I am looking at the conservation part of the molecule. This is what — if I'm going deeper into the problem. That what I'm looking for — I'm seeing that I — well I have an ethyl group here. I found it back on the other side here.

R Uh huh.

A Um so what else is changed in this? I have a one, two, three, four, five, six-membered ring if I include the oxygen in it. Uh I end up with only a five membered ring on the other one. With um an alkene and two methyl. Um so what is the way I have to obtain such a thing? Um this mean I must have a ring closure to close the ring to a five membered ring. And also to add two methyls in it. I have an aldehyde. Um I don't know if I would be able to solve it very fastly. I'm not sure at all. Um the aldehyde — um the double bond isn't very easy. When the double bond in the end of the material. This is not very easy to consider as it's written upside down. Referring to this one. So I'm going to write this the same way um the product is written on the paper. So H and O. There we are. So I end up with this one. So this is conserved. This is also. This is. So I have migration of the double bond. (s1, p. 5)

After choosing the second set of compounds to work with, Andrew correlated the functional groups in the starting material and the target compound. He saw a very strong correlation between the ethyl groups which led him to redraw the structure.

C ... So I got to find a way to close this. Ok, first before I should spend any time, any more time on trying to obtain this intermediate, I had better find a way if I get this that it's going to close. (s3, p 3)

Chuck showed a behavior related to consolidating resources — determine whether a sub-goal is useful and relevant to a problem. Chuck realized that it might be helpful to determine the usefulness of an intermediate before he devoted more time to suggesting a synthesis for it. This was one of the few explicit resource-allocation heuristics that a subject displayed while solving these tasks.

C I don't have any real preference. I'm just gonna go for the first one. Let's see, cyclobutene, substituted cyclobutene converted to a fused six and five membered ring. Now, fused five and six membered ketone. With a — ok, let's see. I'm I'm gonna take a shot and count up the carbons here. It looks like it could be a hidden dimerization of some kind. I don't know. Four, five, six and the final product a has six, seven, eight, nine, ten carbons. (s3, pp. 10-11)

Chuck pointed out an algorithm that he sometimes uses while solving synthesis problems — look for possible doubling of carbon atoms.

D Oh let's see. Let's work this one and see what a — let's work on the second one here and see what a I can see. Figure out. Ok. I was thinking about an alpha alkylation here going back to the enolate.

R Uh huh.

C But I don't think that would work. You'll have problems because this methyl ketone over here is, you know, more kinetically acidic. So that's that's not going to work well. Ok. This this a alkylation at the beta position by like conjugate addition I don't think is going to work very well. Because you could be forming a a quaternary carbon beta to the carbonyl group which isn't, isn't a, isn't common.

R Uh huh.

D I mean, you can do it with cuprates, but. You'd also make — have to make the alkyl copper compound when you've got a carbonyl in the group. (s4, pp. 5-6)

Dan explored various paths after choosing his target structure. He generated a possible precursor and then determined how well various methods would work in the forward direction.

E ... So — I'm just going to number the carbons here so I know where I want to put these things at.

R Ok.

E It might not be where they end up at eventually. But it gives me some kind of reference. Two, three, four. Ok. (s5, p. 11)

Numbering several carbons was one way Elton kept track of portions of molecules.

G In that case I have a four membered ring with a double bond. Cannot remember very well — but try to see that. I have a four membered ring with a double bond. And I had a diene can go here, can go here. I would get a four membered ring with a double bond. Cyclobutane butene. Now how is cyclobutene like this? I would form — I would possibly form the diene there. Now is it allowed? Oh well, no. Never mind. It's uh dis con — so no problems. Allowed thermally. So — well — in a synthesis I can do whatever I like. If I want to make the uh photolysis — I mean photochemistry, it's ok. (s7, pp. 7-8)

Glen realized that he would have to open the ring, and used physical principles to guide this step. He also used another heuristic — work a process on a simpler system — to examine this ring-opening step (i.e., comparing his system with cyclobutene).

E Ok. I'm just going to write it all out at once so I can make sure it is right. Ok so we start with phenol. And use like um (Pause) — it has to be some kind of aprotic a solvent. Because somehow — I don't know. Some kind of ketone. Say something like that.... Yea. Reprotonating. To make it form the quinone. And it gives you a negative center here. And you would just actually put the halogen probably in this. Two, three, four. That might actually even do it all in one step.

R Yea. It seems it would keep

E Because it would just keep going back and forth — flipping back and forth until you got the whole thing.

R Uh huh.

E But anyway for an intermediate you would have something like that. And this would — the negative would attack and flip everything through. And give you mono — see one, two, three, four — and the other halogen here. And then the base is still going to go back and flip back and forth. And give you the product finally. Ok. Now what is that? That's — yea that's right. Ok?

R Ok.

E And then let's see. Still going to have that extra double bond in there, right?... So the only problem we have is that double bond. (s5, pp. 18-19)

Elton decided that his approach was not too bad. At that point he summarized his solution and in doing so realized that he had not reduced one of the double bonds.

J Ok so let me think of uh ethyl bromide. First of all let me get the anion from my cyclohexanone.

R Ok.

J Do with base. Ok now if I have ethyl bromide (Pause). Ok now wait a minute. Is that what I want? That's correct. Let me go go ahead and react this with ethyl bromide, Et. I would have to worry about alkylation at both alpha sites.

R You know of any ways you can control that?

J Well (pause) by making certain that I have a very small concentration of — oh ok let me see how I want to do this. I would have a reagent container of base. [Draws reaction vessel.] And if I dropped in the ketone slowly it would react — oh ok first of all let me think of what I want to avoid. I want to avoid having a whole bunch of this species, the monoalkylated species, around. I would prefer to always keep a very low concentration of this anion. So I'd somehow arrange to do that. Perhaps by having concentrated base and dropping in the ketone. That would control — to make certain that I have monoalkylation.

R Uh huh.

J Let's see what what is my starting material? Let me draw that here. And the — well I really probably need to consider the sequence I do these things. Should I ethylate first and then methylate? Or methylate and then ethylate? And I'm not too sure how — maybe in this case it wouldn't make a difference. Now if I react this with a base — now let's see, what conditions do I want here? Kinetic conditions because I want to abstract the most easily abstractable proton. Which would be this one. This is the thermodynamic proton here which I want to avoid. No, now wait a minute. Is that right? Oh just a second. No no, ok no. I was thinking that the other — that I was interested in alkylating this site. I'm not. So what I just said was incorrect. Let me look at what I have. At this point I have this. I'm trying to get to this product. (Pause). Actually I would like to attack the carbonyl with a reagent to give me the alcohol. Ok I want to attack the carbonyl with a methyl reagent, well a methyl something. (s10, pp. 5-6)

Jane thought about what she would do in the laboratory to guide key steps in her solution. In addition, it occurred to her that she had a choice of sequences to consider. Jane considered whether the order of alkylation might affect her pathway, and used physical principles to determine what might be added and at what time. She also realized she was forming a bond in the wrong place. Throughout this process she continued to ask herself questions.

L	Um ok. First thing -- normally six rings -- the best way to make six rings is Diels-Alder reaction or Robinson annulation, or say Birch reduction. And this kind of reminds me of Diels-Alder reaction. For example if I take some diene -- um I can actually disconnect this. That would be the best thing to do. So if this part is a diene, and if I can get this, some kind of dienophile, then that would work I think. Let's see. If I can get butadiene here and uh -- hm. This is a problem. That won't work.

R	Why not?

L	If I take this part of butadiene it will give double bond this side. Uh not here. (s12, p. 6)

Leon started task 1 by pointing out that there are several ways to form six-membered rings. He disconnected the target molecule so he could see the intermediates required for a Diels-Alder reaction. Leon then examined potential difficulties with the reaction.

Evaluation — Task 4

As with the preparation tasks, the subjects showed similar behaviors while solving the evaluation task. They usually began by following through the pathways to see if they "made sense". After working through the pathways they would use various criteria to determine which pathway was the "best" solution. The criteria included the yield of individual reactions and the overall yield of the pathway, the difficulty of carrying out certain reactions or separation techniques in the lab, the number of steps in the pathway, the stereocontrol employed throughout the path, the cost of some of the reactants, and being able to understand the chemistry in the pathway.

Below are excerpts illustrative of the processes described above.

A	Well the first thing if I have such a molecule the first thing I would look is the yield. I think this is the first reference um for the -- I have step for the first one. 100, 86, 81, 54 -- this is not good at all -- and 60 percent yield. For the second one 80, 92, 97, 30. Ok. So if I already want to know what the final yield should be so um it should be -- this is a matter of calculation. I have never done this before so I have to think about a little bit about it. Anyway well as the first step I have one step less on the first part -- on the second part. But at the first step is 100 yield. For the first one is only an manipulation -- well uh assuming we are not too lazy. Um this isn't a problem. So 86 for 80, 81

R	Uh I think that one's 91.

A	91 yea yea this is. Uh so your -- their uh rel related steps. Um the first two are roughly the same. The third one is far better for the second. But on the other hand is not so good. So for the yield they are roughly the same.... So I'm not going to look at this. Manipulations I have one more step in the first one. Maybe they have written not all -- no they are all written. So there is no tricks for -- I mean no hidden material.

So there is only one more step for the first one. So I am ending with four more percent for one more step. Uh now I think I have used up all the way I know to do it.

R Uh huh.

A Um now -- the recently -- which is the the best? The best um means uh -- I don't -- maybe I don't have enough information. Because the best is also a question of time I think. Um there is no time written. Maybe the first step of the first reaction is going to take a week.

R Uh huh.

A This is possible. Um let's look -- as I have no information with the time. Oop I have a chromatography here. Um the first one has no chromatography. This mean that um -- this is always -- I I had in one of my projects to do chromatography.... I don't -- I'm not one hundred percent enantioselective. This is always the case anyway.

R Uh huh.

A Um so well always -- about always. Well I would say that this one has two inconveniences. The use of chromatography twice. And also the starting material here. The R naphthyl so on must be a very expensive starting material.

R Ok.

A It's already an optically active material. It doesn't sound like a natural one. Maybe it is. If it's natural maybe it's cheaper.

Andrew began task 4 by examining the stepwise and overall yields of the two pathways. He went on to consider the number of steps in each path and question what is meant by the "best" synthesis. He then pointed out that one of the pathways contained a separation procedure that he did not like. Andrew summarized his choice by explaining that chromatographic separation was inconvenient and that the optically active starting material in the second pathway might be expensive unless it was a natural product.

C Ok let's see, first the beta hydroxy group is protected with. I don't understand this this um protective group. Let's see.

R They're protecting this and then reducing this.

C LAH ok. I didn't read the whole thing. Ok, first step is -- just trying to get the protective group here.... Catalyzed with toluene sulfonic acid. Followed by LAH reduction of the carboxylic -- of the ester, to the corresponding alcohol. Retaining the stereochemistry at the two carbon -- there should be no reason for it to change.... I don't I don't know if I'm going about this right. I'm almost checking what they're doing.... Well, I mean right away I I think I'm going to say the first route is better. It's very stereocontrolled throughout the whole thing. All the stereochemistry was taken care of before the cyclization.

R Um huh.

C Now if I was to add up -- should I go through and do all these yields here?

R They come out to be, I think this one's 24 percent and this one's 21 percent. So not really that different.

C Um ok. Well for, I'm gonna say for that reason because the very last step here there's just no regio -- stereocontrol over where the alkylation is going. (s3, pp. 15-21).

Chuck began task 4 by working through the chemistry of the two pathways. He suggested the first pathway was better because it was stereocontrolled. Chuck decided that the yield of the two paths was unimportant in his decision because they were about the same. In addition to choosing the first path as the better of the two due to its stereocontrol, he discounted the second pathway because of the lack of stereocontrol during the alkylation of the lactone.

J Ok, we've protected the alcohol and reduced the ester. Um did a displacement. Oxidized. Ok. So then this attacks here. Opens that up. Is this sodium

R Mercury.

J Mercury? Ok. You get the anion. Acetylate it. That must have taken off your THP. Ok and then reduced, I mean oxidize. Form the lactone.

R What was that look about?

J I never -- this is something new to me. I'm not familiar with this. Um isocynate?

R Isocynate, right. And then form the carbamate. (Long pause).

J Ok um so this is attacking this. This is attacking (Long pause) I guess here, huh?

R Right.

J Ok. Chromatography. Ok then silate. Ok. I have to see what's going on here. I guess I would wonder with this particular reaction if um -- it looks like this one is more stereoselective because you introduce this already. Where if you're methylating here, how do you know if it's going to be cis or trans to the other methyl

R Right.

J group? So I I would choose this one over this one.

R Top one cause it set up the stereochemistry? Are there any -- when you're doing work of your own, how do you decide whether a synthesis was better than another pathway you could have chosen?

J Well you also look at steps too. One, two, three, four, five. One, two, three, four. I guess you're looking at only four here.... None of these reaction look like they would be too hard to perform so one more step may not be that big of a problem. (s11, p. 10-14).

Like the other subjects, Jane began by working through each of the pathways to try and understand the chemistry used. She then rated the first pathway as better because it was more stereoselective while the alkylation of the lactone in the second path was uncontrolled. When asked about using different pathways in her own research she went on to comment that she also looks at the total number of steps and the difficulty in performing the reaction.

L This is really beyond my capacity to uh criticize but yea. Hydrolysis (laughs). That makes sense. That is really easy. Hydrolysis gives acid and lactonization. Yea yea ok that will give here. Then this one -- ok same thing. If I treat it with LDA -- now cyanide is good as.... Uh I doubt -- this chemistry I'm not really familiar with uh the second problem so. Uh the first one -- at least everything made sense to me. Um adding some of my own. But yea that should work. I mean as far as I know.

R Uh huh.

L And uh about this uh both give the same compound. The second gives in 30 percent.

R Uh these are stepwise yields.

L Step oh ok.

R Overall yield is 24 for the first one and 21 for the second one,

L Ok. Um let's see -- how many number of steps? This I think has the less number of steps. Three four. Five. Um -- yea. This is kind of formulaic chemistry. Very easy to do. And reagents are available.

R Uh huh.

L So depends on that also. Like I don't know whether this reagent is available commercially. (s12, p.27).

Leon began task 4 by working through each reaction in the two paths to see if they made sense. He then went on to examine the yields and the number of steps involved. He also considered how difficult the reaction would be to perform and whether the chiral starting material was commercially available. Unlike the other subjects, Leon did not suggest that the first synthesis was better because of stereocontrol. He appeared to be most concerned with whether he understood the chemistry.

A Summary of Problem Solving Behaviors

The previous excerpts have illustrated various behaviors graduate students display while in the various stages of problem solving. The purpose of this section is to give a summary description of how graduate students solve tasks related to synthesis.

Bowen (in press) found that graduate students used different representational systems while solving tasks in organic synthesis. He defined a representational system as a collection of interrelated concepts and processes that a problem solver uses to solve a problem and communicate the solution to others. Seven representational systems were identified: Verbal, pictorial, methodological, principles-oriented, literary, laboratory, and economic. Subjects primarily used the verbal, pictorial and methodological representations while solving synthesis tasks.

Graduate students solve synthesis problems similar to the model described by Bourne et al. However, instead of preparing for the entire problem, preparing an entire solution, and evaluating the solution all at once, graduate students use each of these phases in small steps. In each of these phases they use a different representational system. After proposing a step in the solution (usually a reaction), the graduate student evaluates it by deciding whether the proposed reaction would work and whether it was worthwhile to continue along the pathway.

Subjects begin problem solving in organic synthesis by deciding which representational system provides a useful framework for problem solving. For the most part the choice of representational system is made without conscious thought. During the preparation stage the problem is represented in verbal and pictorial terms. Subjects seek relationships between the verbal or pictorial representation and a relevant representation in the methodological system. The initial functional groups that are identified are correlated to specific reactions in which the desired functional groups is formed (e.g., six-membered ring suggests using a Diels-Alder approach). The beliefs subjects have about useful ways of thinking in organic synthesis guide their choice almost exclusively to the methodological framework for the production phase of problem solving. After generating a step in their solution (i.e., a reaction) they might evaluate it using another representational system such as the literature, chemical or physical principles, or a laboratory approach. For example, they might look up a similar reaction in a book, or try to rationalize the outcome of a reaction on kinetic or thermodynamic grounds.

A Model of Problem Solving

For this study it was assumed that problem solving takes place in the way described by

Bourne et al. The problem solver begins by preparing for the problem by constructing a representation of the problem based on his own knowledge and its interaction with the problem. After constructing a representation of the problem the problem solver moves into the production stage. This stage is where the problem solver generates a solution based on his representation of the problem. The problem solver then evaluates the solution (or the partial solution). The problem solver cycles through these stages until the problem is solved.

Schoenfeld (1983) described a way to think about the decision-making processes that people use while problem solving that is not incompatible with the model described above. In fact, I think it is a useful way to extend that model. He said that decision-making processes can be categorized into two areas.

> Two qualitatively different kinds of decisions, tactical and strategic, seem to be needed for problem-solving success in broad, semantically rich domains.... Here, *tactics* include most standard procedures for implementation in problem solving. Tactics include all algorithms and most heuristics, both of the Polya type (e.g., draw a diagram whenever possible; consider special cases) and of the kinds used in artificial intelligence (means-ends analysis, hill climbing). Tactical decisions are "local".... In contrast, **strategic** decisions are those that have a major impact of the direction a solution will take, and on the allocation of one's resources during the problem-solving process. These will also be called **executive** and **managerial** decisions. For example, if one is given 20 minutes to work on a problem, and calculating the area of a region is likely to take 10 minutes, the decision to calculate the area of that region is strategic — regardless of whatever particular method is chosen for performing the calculation. Like a decision during wartime to open a front, this one choice may determine the success or failure of the entire enterprise (pp. 345-346).

Schoenfeld's dichotomy of decision making provides a useful way to examine problem solving that is compatible with the three-stage model described by Bourne. What follows is a model of problem solving in organic synthesis that incorporates both of these models. I believe that one of the most important strategic decisions involves determining the representational system to use while solving the task at hand. These graduate students used different representational systems when they were in different stages of solving the tasks. For the most part the choice of representational system to use for a given problem-solving stage was made with little conscious thought. Movement between the representational systems was also automatic. The choice of a representational system is a strategic decision that can greatly influence success in any of the phases of problem solving.

When examining the protocols patterns of choices of representational systems emerge. The representational systems that students chose to use (either consciously or unconsciously) appeared to be related to the stage of problem solving they were in. Figure 1 summarizes these correlations. In all three stages of problem solving the students used the verbal and pictorial systems of representation. The methodological, literary, and laboratory representational systems were used in the production stage. During the evaluation stage the students used representations grounded in principles, the literature, laboratory knowledge and economics.

Tactical decisions are found within the representational system that the problem solver chooses to work in. For example, in the pictorial representational system the problem solver decides which type of pictorial representation might be most useful to solve the task (e.g., a Lewis structure, Newman projection, or wedge structure). Another example involves the choice of tactic the problem solver makes when using the literature of organic chemistry. How does the problem solver use the literature for the task at hand? Does he or she use Chemical Abstracts, Science Citation Index, Organic Reactions, or does he or she try to go directly into the primary sources? The problem solver uses the tactics within the representational system for various stages in the problem-solving process.

Implications for Instruction

In the previous section it was suggested that graduate students solve problems in organic synthesis by 1) choosing a representational system depending on what stage of problem solving is being worked on, and 2) choosing tactics within the representational system that might be useful in solving the problem. Although the choice of tactic to use from a representational system is usually made consciously, the choice of representational system is not. Bowen (1988) suggested that teachers should consider helping students learn to do the following:

1) Choose useful representational systems for a problem (or a portion of a problem)
2) Select useful tactics within the representational system for solving the problem (or portion of the problem)
3) Abandon a representational system if it does not provide a solution, yet consolidate gains to decide what to do next
4) Evaluate a solution (or portions) by using multiple representational systems (p. 284).

For the most part students select a representational system without much thought. One of the strategies that teachers could help students learn is what representational system might be useful for a given portion of a problem. The teacher has expertise in the field which allows him or her to decide what ways can be useful for solving a problem. The decision-making knowledge about problems in a domain might be explicitly modeled to help students learn how to use different representations effectively.

Most of the instruction in the classroom of the students involved in this study involved helping students learn a great deal of information that might be useful in synthesis. At times it seemed like a catalog of information. What was not as clear, yet probably more concrete than choosing a representational system, was how to choose a tactic within a representational system. Teachers might consider how they choose a tactic while solving problems and try to help students learn what to do while making such choices.

Occasionally a representational system will fail to be useful in aiding the problem solver in constructing a solution for a problem. Teachers might consider helping students learn what to do when a given representational system fails. A representation might not be totally useless but some information might be salvaged that can be used to decide what to do next. If students are helped in constructing relationships between representational system, then they might see what they might consider trying next.

Evaluation of a solution, or a portion of a solution, was an area that the students could use improvement. On the local level (i.e., after each proposed reaction) students occasionally used concepts and processes from other representational systems to determine how well a step in the solution would work. For the most part evaluation did not take place at a global level to see how good the entire solution was. Teachers might assist students by convincing them of the power of using multiple representational systems while evaluating a solution (e.g., chemical principles and literature precedents can add to the credibility of a reaction proposed from the methodological system).

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